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A STUDY OF NORDSIECK-TYPE PREDICTOR-CORRECTOR METHODS

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A Study of Nordsieck-type Predictor-Corrector Methods

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1. Introduction

Today, one common type of problem being solved on computers is the numerical integration of the initial value problem

$$\vec{y}' = \vec{f}(x, \vec{y}) \quad \vec{y}(x_0) = \vec{y}_0 . \quad (1.1)$$

Although there exist specialized techniques for solving such problems, the two most commonly used are the single step (e.g., Runge-Kutta) and multistep (e.g., Adams) methods. The major advantage of the multistep methods over the single step methods is that fewer functional evaluations are usually required per integration step. For this reason, the authors will limit the discussion that follows to predictor-corrector schemes.

For the individual who wants a solution to (1.1), there are two important considerations when selecting a method: speed and accuracy. For the researcher who is developing a predictor-corrector procedure, there are three important considerations: speed, truncation error and stability. The basic factor for determining speed is the number of functional evaluations required per step. Accuracy is determined by the stability error and truncation error of the method. The Adams methods have been shown to be about as good as any of the existing predictor-corrector formulas. The major problem with these formulas is that interval modification and interpolation are difficult. Nordsieck [1] has devised a method equivalent to one of the Adams

methods which accomplishes these tasks simply and inexpensively (Appendix C). Also, Nordsieck's method has a built-in automatic starting procedure, a feature not available with the Adams formulas.

2. The Methods

The derivation of Nordsieck's method is based on Taylor's theorem. The authors refer the reader to Nordsieck's paper for a detailed description of the method. Nordsieck stores the current values of the higher derivatives of a polynomial approximating the solution. Adams stores successive values of a polynomial approximation for $\vec{f}(x, \vec{y})$ at several backward points. Nordsieck saves the equivalent polynomial information as Adams but in a more convenient form for interpolation and interval modification.

The formulas discussed in detail by Nordsieck are equivalent to the 5th order Adams-Bashforth predictor and the 6th order Adams-Moulton corrector. Descoux [2] has derived a Nordsieck-type formula which is equivalent to the 6th order Adams-Bashforth predictor and the 6th order Adams-Moulton corrector. The authors will study these particular formulas because of their desirable stability and truncation error properties. The following terminology will be adhered to: the original formulas derived by Nordsieck will be called the standard Nordsieck formulas; the formulas derived by Descoux will be called the modified Nordsieck formulas. These equations written in terms of backward points are given in (2.1) and (2.2).

Standard Nordsieck

$$\begin{aligned} \text{predictor: } y(x+h) = y(x) + \frac{h}{720} (1901f(x) - 2774f(x-h) \\ + 2616f(x-2h) - 1274f(x-3h) \\ + 251f(x-4h)) \end{aligned} \tag{2.1}$$

$$\begin{aligned} \text{corrector: } y(x+h) = y(x) + \frac{h}{1440} (475f(x+h) + 1427f(x) \\ - 798f(x-h) + 482f(x-2h) \\ - 173f(x-3h) + 27f(x-4h)) \end{aligned}$$

Modified Nordsieck

$$\begin{aligned} \text{predictor: } y(x+h) = y(x) + \frac{h}{1440} (4277f(x) - 7923f(x-h) \\ + 9982f(x-2h) - 7298f(x-3h) \\ + 2877f(x-4h) - 475f(x-5h)) \end{aligned} \tag{2.2}$$

corrector: same as standard Nordsieck corrector

The corresponding equations derived by Nordsieck and Descloux are given in Appendix A.

The reason for studying the modified Nordsieck formulas is that a step by step check on the local relative truncation error can be made. No estimation of the local relative truncation error is available with the standard Nordsieck formulas.

When selecting a predictor-corrector scheme, one must decide the number of corrections (and evaluations) to be made after doing the initial prediction. This is of importance since this choice affects the stability and truncation error of the method. If one iterates to convergence then only properties of the corrector influence the result.

Because it is generally considered that functional evaluations are the most expensive part of the predictor-corrector procedure, the authors will limit the number of functional evaluations to two per step and test only the following procedures: PEC, PECE and PECEC. (P stands for predict, E stands for evaluate and C stands for correct.)

3. Truncation Error

For the single equation $y' = f(x, y)$, we use the notation:

$y(x)$ = true solution of the differential equation

$y_n(x)$ = Nordsieck solution for $P(EC)^{n-1}$ or $PE(CE)^{n-1}$

$\delta_n(x) = y_n(x) - y(x)$

$f_n(x) = f(x, y_n(x))$

$y_p(x)$ = predicted value of y

$f^p(x)$ as defined by Nordsieck

h = the stepsize.

The Nordsieck iteration for one step from x to $x+h$ is then

$$y_1(x+h) = y_p(x+h) \quad (3.1)$$

$$y_n(x+h) = y_p(x+h) + \frac{95}{288} h(f_{n-1}(x+h) - f^p(x+h)), \quad (3.2)$$

$n \geq 2$

The error for the standard Nordsieck is

$$\delta_2(x+h) = \frac{863}{60480} h^7 y^{(7)}(x+h) - \left(\frac{95}{288}\right)^2 h^7 y^{(6)}(x+h) \frac{\partial f}{\partial y}(x+h, y(x+h)) \quad (3.3)$$

$+ O(h^8)$

$$\delta_n(x+h) = \frac{863}{60480} h^7 y^{(7)}(x+h) + O(h^8) \quad n \geq 3 \quad (3.4)$$

and the error for the modified Nordsieck is

$$\delta_n(x+h) = \frac{863}{60480} h^7 y^{(7)}(x+h) + O(h^8) \quad n \geq 2. \quad (3.5)$$

In the standard Nordsieck case we know

$$f_n(x+h) - f^p(x+h) = h^5 y^{(6)}(x+h) + O(h^6) \quad n \geq 1 \quad (3.6)$$

$$y_n(x+h) - y_p(x+h) = \frac{95}{288} h^6 y^{(6)}(x+h) + O(h^7) \quad n \geq 2 \quad (3.7)$$

$$y_3(x+h) - y_2(x+h) = \left(\frac{95}{288} \right)^2 h^7 y^{(6)}(x+h) \frac{\partial f}{\partial y}(x+h, y(x+h)) + O(h^8). \quad (3.8)$$

$$f_2(x+h) - f_1(x+h) = \frac{95}{288} h^6 y^{(6)}(x+h) \frac{\partial f}{\partial y}(x+h, y(x+h)) + O(h^7). \quad (3.9)$$

No satisfactory measure of $y^{(7)}$ exists. However in the modified Nordsieck case we have the information

$$f_n(x+h) - f^p(x+h) = h^6 y^{(7)}(x+h) + O(h^7) \quad n \geq 1 \quad (3.10)$$

$$y_n(x+h) - y_p(x+h) = \frac{95}{288} h^7 y^{(7)}(x+h) + O(h^8) \quad n \geq 2. \quad (3.11)$$

Thus, in this case, an approximation for $\delta_n(x+h)$ is

$$\delta_n \approx \frac{863}{19950} (y_n(x+h) - y_p(x+h)) \quad n \geq 2. \quad (3.12)$$

For a system of m equations

$y_i' = f_i(x, y_1(x), \dots, y_m(x))$, $i = 1, \dots, m$, we use the notation:

$y_i(x)$ = true solution of the differential equation

$y_{i,n}(x)$ = Nordsieck solution for $P(EC)^{n-1}$ or $PE(CE)^{n-1}$

$\delta_{i,n}(x) = y_{i,n}(x) - y_i(x)$

$f_{i,n}(x) = f_i(x, y_{1,n}(x), \dots, y_{m,n}(x))$

$y_{i,p}(x)$ = predicted value of y_i

$f_i^p(x)$ as defined by Nordsieck.

The error for the standard Nordsieck is

$$\begin{aligned} \delta_{i,2}(x+h) &= \frac{863}{60480} h^7 y_i^{(7)}(x+h) \\ &\quad - \left(\frac{95}{288}\right)^2 h^7 \sum_{j=1}^m y_j^{(6)}(x+h) \frac{\partial f_i(x+h, y_{1,n}(x+h), \dots, y_{m,n}(x+h))}{\partial y_j} \\ &\quad + O(h^8) \end{aligned} \quad (3.13)$$

$i = 1, \dots, m$

$$\delta_{i,n}(x+h) = \frac{863}{60480} h^7 y_i^{(7)}(x+h) + O(h^8) \quad n \geq 3 \quad (3.14)$$

$i = 1, \dots, m$

and the error for the modified Nordsieck is

$$\delta_{i,n}(x+h) = \frac{863}{60480} h^7 y_i^{(7)}(x+h) + O(h^8) \quad n \geq 2 \quad (3.15)$$

$$i = 1, \dots, m.$$

Equation (3.12) now becomes

$$\delta_{i,n} \approx \frac{863}{19950} (y_{i,n}(x+h) - y_{i,p}(x+h)) \quad n \geq 2. \quad (3.16)$$

4. Stability

The necessary theoretical background on stability can be found in the papers by Krogh [3], Crane and Klopfenstein [4] and Chase [5]. By examining the eigenvalues $\{\lambda\}$ of the Jacobian matrix of \vec{f} with respect to \vec{y} , the stability of a method can be investigated. It will be assumed that the Jacobian matrix is completely diagonalizable and the eigenvalues are approximately constant over an interval of $5h$ (standard) or $6h$ (modified). The authors have some evidence that the results in this section hold for Jacobian matrices which are not completely diagonalizable. Consider the set $\{s : s = h\lambda\}$. The values of the elements of this set determine whether or not the method remains stable. Briefly, a method is absolutely stable if errors decrease in magnitude. A method is relatively stable if errors do not grow more rapidly than the solution.

Formulas given by Hall [6] allow the computation of the characteristic equations

$$p(z,s) = 0 \quad (4.1)$$

for the standard and modified Nordsieck PEC, PECE and PECEC algorithms (Appendix B). With the appropriate conditions [3,p.380] applied to these equations, the absolute and relative stability diagrams have been computed (figures 1-5). Because of the symmetry involved, only the upper half of the s-plane is given in each diagram. The heavy solid curves bound the absolute stability regions. The portion of these curves which appears to coincide with the imaginary axis is just very close to it. The area to the right of the dashed curves is the region of relative stability. In the right half s-plane, this region does not have a well-defined boundary. Examination of the five diagrams yields the following two results:

- 1) the diagrams for both the standard and modified Nordsieck formulas decrease in area in the following order: PECE, PECEC, PEC;
- 2) the standard Nordsieck PEC, PECE and PECEC diagrams are larger than the modified Nordsieck PEC, PECE and PECEC diagrams respectively.

Although diagrams for different order Adams formulas have not been computed, the same general result is expected.

An example will show that absolute stability will not always insure an accurate solution. The stronger condition of relative stability will be required. The definition of relative stability presented by

Krogh [3,p.377] is as follows:

Defn. For $|s|$ sufficiently small, one of the roots (of the characteristic equation (4.1)) r_p , the principal root, is approximately e^s . Any other root we label r_e to indicate that it is extraneous. If each of the r_e satisfy $|r_e| \leq |e^s|$, and if the r_e with magnitude of e^s are simple, then a method is said to be relatively stable.

Example. Problem: $y' = -y$, $y(0) = 1$

Solution: $y(x) = e^{-x}$, $\lambda = -1$

Procedure: standard Nordsieck PEC with constant s

<u>Absolute Value of Relative Error</u>		
<u>x</u>	<u>s = -.07</u>	<u>s = -.08</u>
3	.571-5	.116-4
6	.486-5	.272-4
9	.524-5	.120-3
12	.533-5	.251-3
15	.547-5	.252-2
18	.561-5	.656-2
21	.574-5	.620-1
24	.584-5	.159-0

Inside the relative stability region ($s = -.07$), the standard Nordsieck PEC calculates a good solution. However, outside the relative stability region but inside the absolute stability region ($s = -.08$) the solution blows up. The standard Nordsieck characteristic equation has been solved for $s = -.07$ and $s = -.08$. Below, e^s and the roots are listed. Complex conjugates are omitted.

s	$-.07$	$-.08$
e^s	$.9323938$	$.9231164$
r_1	$.9323940$	$.9231166$
r_2	$-.9135050$	$-.9632736$
r_3	$-.3054155 + .14072i$	$.3120278 + .1424621i$
r_4	$-.0811852 + .482849i$	$.089245 + .4942325i$

Since $|s|$ is sufficiently small, in both cases r_1 , the principal root, approximates e^s closely. When $s = -.07$, $|r_2|$, $|r_3|$ and $|r_4|$ are all less than e^s as Krogh has required for relative stability. However, when $s = -.08$, $|r_2|$ is greater than e^s . The root r_2 dominates the solution of the error difference equation [7,p.293] and thereby causes the poor results.

In the right half s -plane, as the real part of s gets larger, e^s "moves away" from the roots of the characteristic equation. When the principal root no longer approximates e^s , then the definition of relative stability can no longer be applied. It is then possible that the h is so large that the truncation error will cause a poor solution to be calculated.

Figure 1. Standard Nordsieck PEC

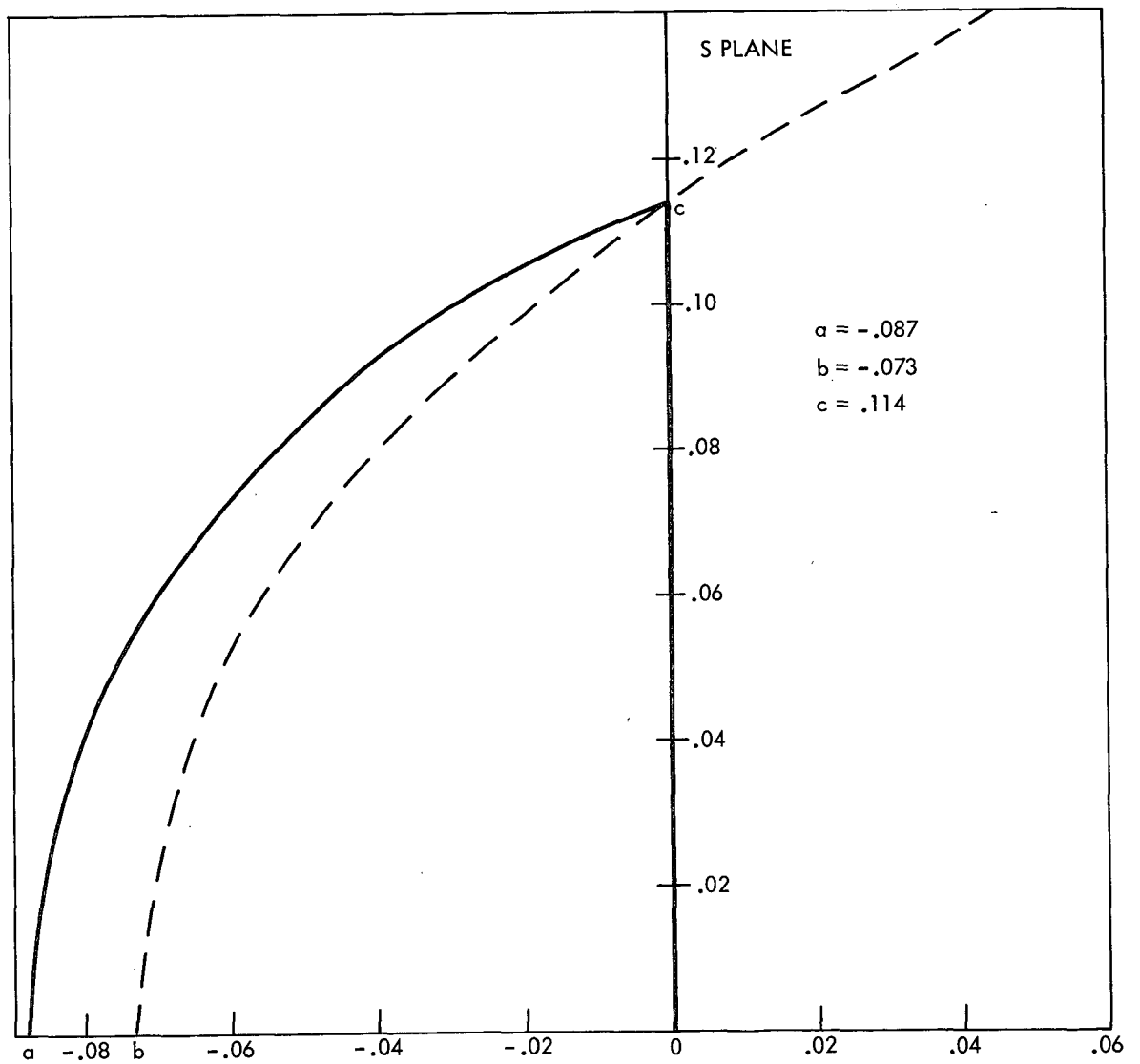


Figure 2. Standard Nordsieck PECE

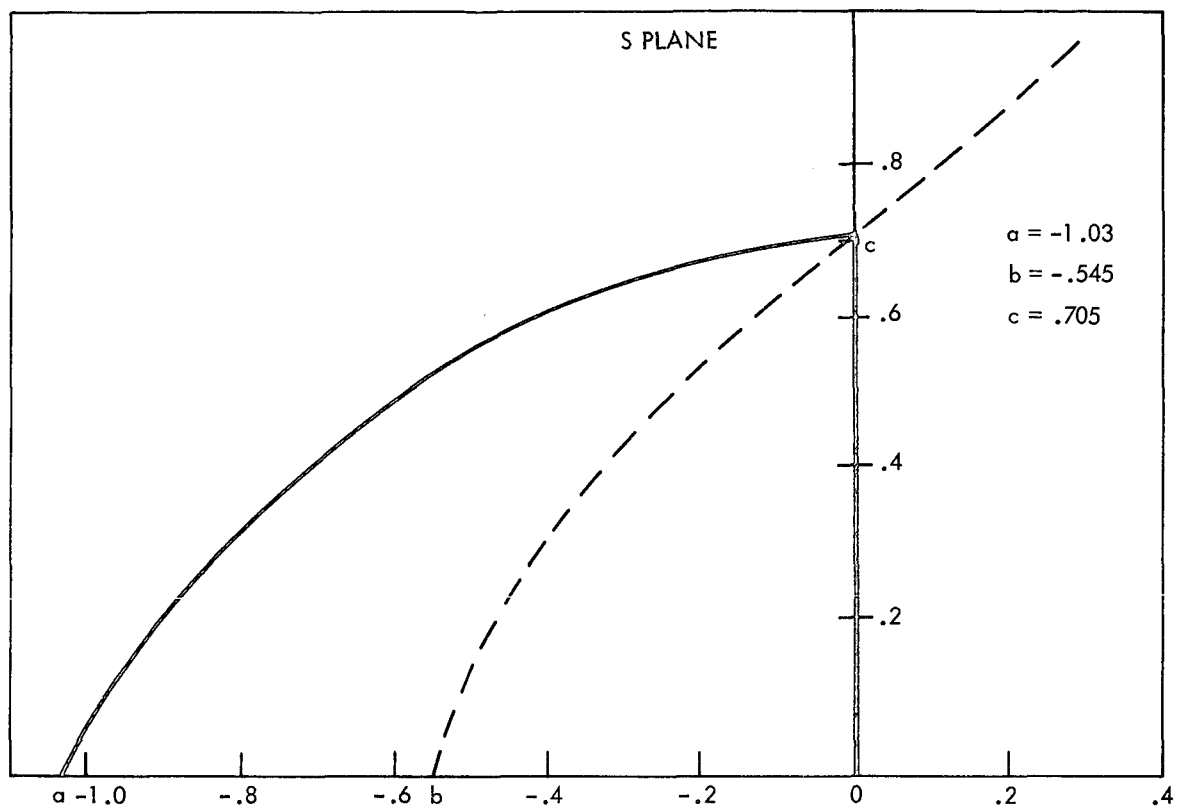


Figure 3. Standard Nordsieck PECEC; modified Nordsieck PECE

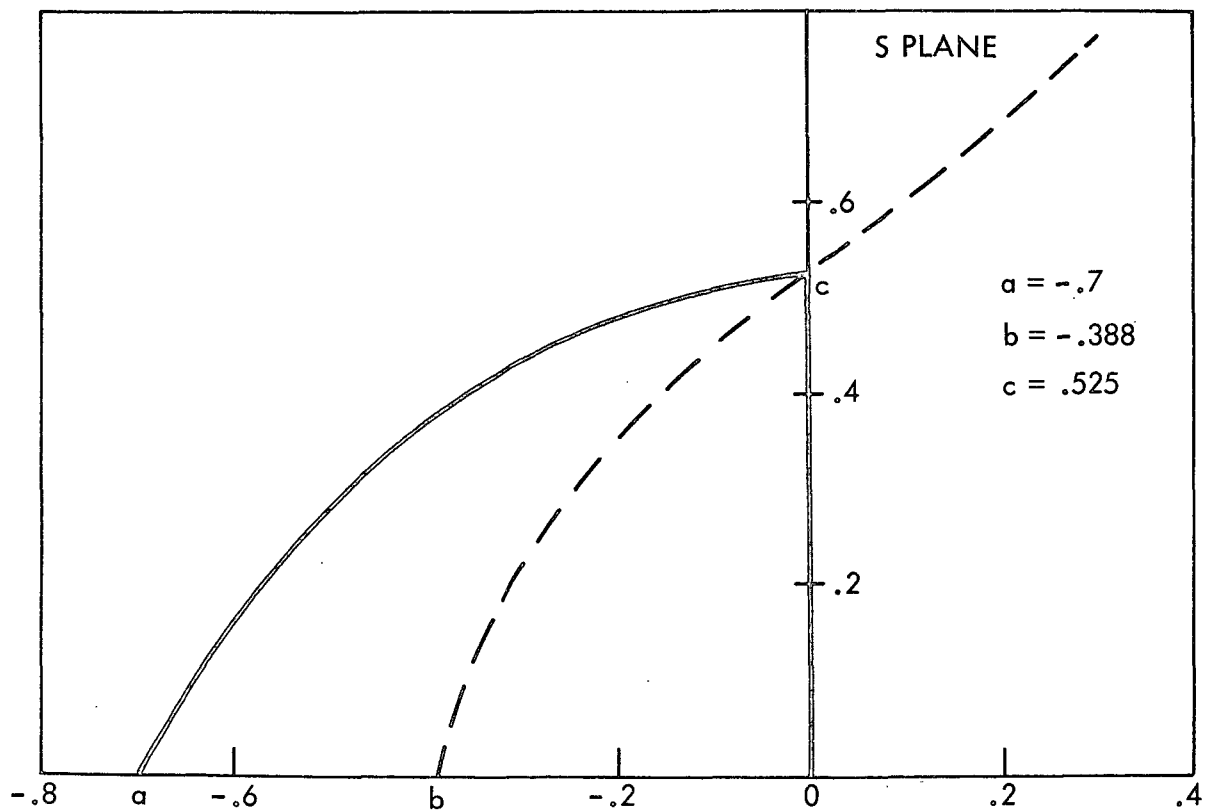


Figure 4. Modified Nordsieck PEC

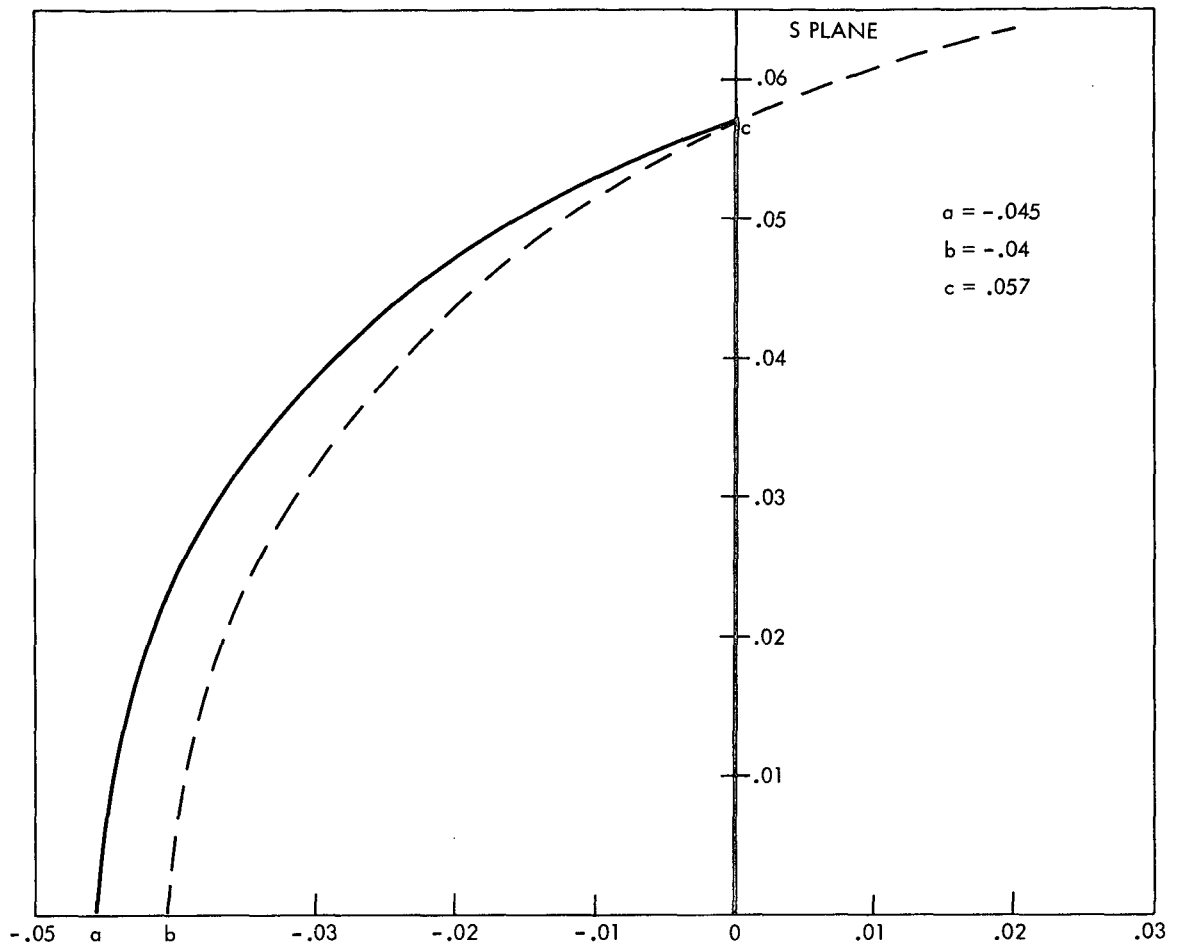
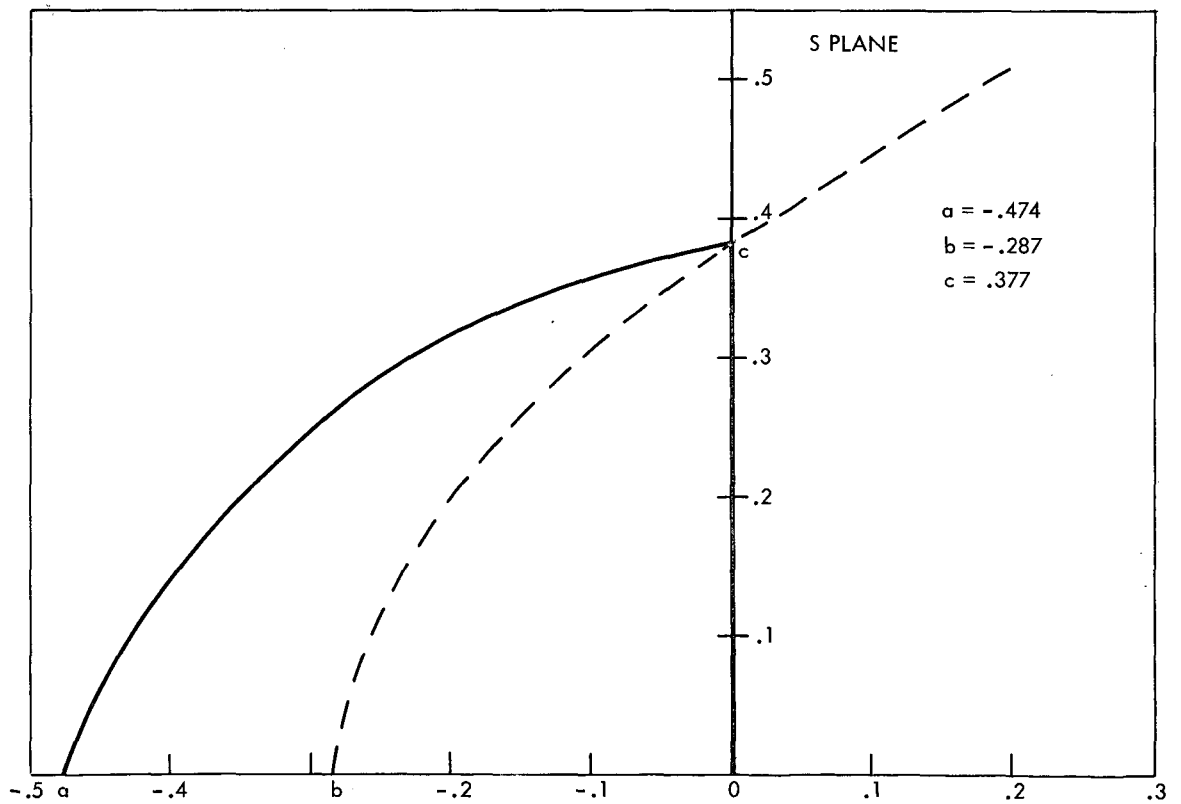


Figure 5. Modified Nordsieck PECEC



5. Computational Considerations

Although the stability diagrams for the standard and modified Nordsieck formulas have been computed, these diagrams are difficult to use in many test problems. The difficulty lies in the fact that an eigenvalue problem must be solved at each integration step. Even if the partial derivatives are known functions or can be closely approximated, the resultant eigenvalues may not be accurate. Matrix norms [8] are available which allow the computation of an upper bound for the moduli of the eigenvalues. However, there is no assurance that these approximations will be reliable. For these reasons, it is desirable to find some way to insure stability at each step without having to consider the values of s . Unfortunately, there is no known technique available to accomplish this for all initial value problems.

Even if the eigenvalues are known, it is the nature of the true solution to the differential equation that determines which values of s are essential to the stability of the problem. Furthermore, the type of stability that is appropriate to consider is also determined by the behavior of the true solution. In many cases, relative stability is too strong a condition to impose to control the stability error.

6. Test Problems

Because of the lack of a minimal comprehensive set of test problems for comparing the efficiency of our algorithms, the authors chose the following examples without claim to the completeness of the selections:

$$1) \quad y' = -y, \quad y(0) = 1, \quad x_0 = 0, \quad x_{\max} = 100, \\ \text{with solution } y(x) = e^{-x} \text{ and } \lambda = -1;$$

$$2) \quad y_1' = y_2, \quad y_1(0) = 0, \quad x_0 = 0, \quad x_{\max} = 20, \\ y_2' = -y_1, \quad y_2(0) = 1, \\ \text{with solutions } y_1(x) = \sin(x), \quad y_2(x) = \cos(x) \\ \text{and } \lambda = \pm i;$$

$$3) \quad y' = 2xy, \quad y(0) = 1, \quad x_0 = 0, \quad x_{\max} = 10, \\ \text{with solution } y(x) = e^{x^2} \text{ and } \lambda = 2x;$$

$$4) \quad y' = -xy(1 + y^2), \quad y(0) = 1, \quad x_0 = 0, \quad x_{\max} = 10, \\ \text{with solution } y(x) = (2e^{x^2} - 1)^{-\frac{1}{2}} \text{ and} \\ \lambda = -x \left(1 + \frac{3}{2e^{x^2} - 1} \right).$$

The initial h for all problems was 1. Total and successful functional evaluations do not include evaluations done in the starting procedure. Since no accurate measure of the truncation error is available for the standard Nordsieck formulas, the authors defined

$$\begin{aligned} \delta_2 &= h(f_1(x+h) - f^P(x+h)) \quad \text{for PEC,} \\ \delta_2 &= h(f_2(x+h) - f^P(x+h)) \quad \text{for PECE,} \\ \delta_3 &= h(f_2(x+h) - f^P(x+h)) \quad \text{for PECEC.} \end{aligned} \tag{6.1}$$

A local relative truncation error test ($|\delta_n/y_n(x+h)| < \epsilon$) was applied to test problems 1, 3 and 4. An absolute error test ($|\delta_n| < \epsilon$) was applied to problem 2. The input values of ϵ for our test programs were 5.0×10^{-4} , 2.5×10^{-4} , 10^{-4} , 7.5×10^{-5} , 5.0×10^{-5} , . . . , 7.5×10^{-17} . No stability requirements were imposed in the test programs. The test problems were solved on an IBM 360/91 using double precision arithmetic.

The results for $\epsilon = 10^{-6}$ and 10^{-13} are given in Tables 1-4. In an effort to make meaningful comparisons, graphs were drawn for each test problem plotting the final accumulated relative error (absolute error for problem 2) versus total functional evaluations for each value of ϵ . These graphs are not presented here.

7. Alternative Interval Modification

An alternative method for determining the stepsize for the modified Nordsieck formulas was developed as follows: Assume that one step has been taken from x to $x + h$. Impose the relative error condition

$$\left| \frac{\delta_n}{y_n(x+h)} \right| < \epsilon. \quad (7.1)$$

Since $\delta_n = \frac{863}{60480} h^7 y^{(7)}(x+h) + \dots$ then an "optimum" interval may be found using the relation

$$\left| \frac{\delta_n}{\epsilon y_n(x+h)} \right| \approx \frac{h^7}{h_{\text{opt}}^7} \quad (7.2)$$

or

$$h_{\text{opt}}^7 \approx h^7 \epsilon \left| \frac{y_n(x+h)}{\delta_n} \right|.$$

Using the approximation (3.12) for δ_n yields

$$h_{\text{opt}} \approx h \left(\frac{19950 \epsilon}{863} \left| \frac{y_n(x+h)}{y_n(x+h) - y_p(x+h)} \right| \right)^{\frac{1}{7}}. \quad (7.4)$$

For m -dimensional systems, let h_{opt} be the minimum of the right hand side of (7.4) over the m equations. A similar analysis will hold for this section if one imposes an absolute error condition in (7.1). The appropriate changes are easily made in (7.4) and in the following strategy table. Numerical results appear in Tables 5 and 6.

Strategy Table

	Nordsieck Strategy	Proposed Strategy
<p>Error test fails</p> $\left \frac{\delta_n}{y_n} \right \geq \epsilon$ $h_{\text{opt}} \leq h$	$h_{\text{new}} = h/2$ <p>Proceed from x</p>	$h_{\text{new}} = \text{sgn}(h) \cdot \max(t h_{\text{opt}} , \frac{h}{2})$ <p>Proceed from x</p>
<p>Error test passes</p> $\left \frac{\delta_n}{y_n} \right < \epsilon$ $h_{\text{opt}} > h$	$\left \frac{\delta_n}{y_n} \right < \frac{\epsilon}{128} \rightarrow h_{\text{new}} = 2h$ <p>Else $h_{\text{new}} = h$</p> <p>Proceed from x + h</p>	$h_{\text{new}} = \text{sgn}(h) \cdot \max(h , \min(t h_{\text{opt}} , 2h))$ <p>Proceed from x + h</p>

t is a constant which satisfies $0 < t \leq 1$.

8. Final Remarks

Examination of the graphs discussed in section 6 revealed that, for high accuracy requirements (input $\epsilon \leq 10^{-9}$), the standard PEC was more efficient than the standard PECE and PECEC procedures and the modified PEC was more efficient than any of the other procedures tested. For the modified Nordsieck formulas, this result held true for both techniques of interval modification. Neither the Nordsieck strategy nor the proposed strategy was clearly superior to the other. Further investigations are needed to determine when single evaluation predictor - corrector methods are more efficient than multi-evaluation methods.

In conclusion, the authors note that subroutines employing Nordsieck's method have been satisfactorily used by members of the Goddard Space Flight Center for the past three years. The ease of performing interval modification and interpolation are the particular features of this method that were found to be most desirable by scientific personnel at this installation.

Table 1. Problem 1.

		starting h	relative error of y at x_{\max}	no. of integration steps	no. of successful evaluations	no. of total evaluations	no. of evaluations to start
std. PEC	$\epsilon = 10^{-6}$	2^{-6}	.220-5	1607	1607	1607	121
" PECE	"	2^{-4}	.656-6	1600	3200	3200	177
" PECEC	"	2^{-3}	.111-6	1597	3194	3196	145
mod. PEC	"	2^{-6}	.888-6	2376	2376	2410	151
" PECE	"	2^{-3}	.141-4	800	1600	1600	181
" PECEC	"	2^{-3}	.574-5	800	1600	1600	181
std. PEC	$\epsilon = 10^{-13}$	2^{-11}	.168-11	25611	25611	25611	201
" PECE	"	2^{-9}	.177-11	25603	51206	51206	337
" PECEC	"	2^{-9}	.181-11	25603	51206	51206	337
mod. PEC	"	2^{-11}	.296-10	6425	6425	6425	251
" PECE	"	2^{-7}	.243-10	6403	12806	12806	341
" PECEC	"	2^{-7}	.217-10	6403	12806	12806	341

Table 2. Problem 2.

		starting h	absolute error of y_1 at x_{\max}	no. of integration steps	no. of successful evaluations	no. of total evaluations	no. of evaluations to start
std. PEC	$\epsilon = 10^{-6}$	2^{-6}	.221-6	327	327	327	121
"	PECE	"	"	"	"	"	"
"	PECEC	"	"	"	"	"	"
mod. PEC	"	2^{-6}	.534-6	330	330	333	151
"	PECE	"	"	"	"	"	"
"	PECEC	"	"	"	"	"	"
std. PEC	$\epsilon = 10^{-13}$	2^{-11}	.737-13	5131	5131	5131	201
"	PECE	"	"	"	"	"	"
"	PECEC	"	"	"	"	"	"
mod. PEC	"	2^{-11}	.343-11	1305	1305	1305	251
"	PECE	"	"	"	"	"	"
"	PECEC	"	"	"	"	"	"

Table 3. Problem 3.

		starting h	relative error of y at x_{\max}	no. of integration steps	no. of successful evaluations	no. of total evaluations	no. of evaluations to start
std. PEC	$\epsilon = 10^{-6}$	2^{-5}	.615-5	1501	1501	1506	105
"	PECE	"	2^{-4}	1501	3002	3010	177
"	PECEC	"	2^{-4}	1499	2998	3008	177
mod. PEC	"	2^{-5}	.470-3	527	527	543	131
"	PECE	"	2^{-3}	518	1036	1044	181
"	PECEC	"	2^{-3}	528	1056	1066	181
std. PEC	$\epsilon = 10^{-13}$	2^{-9}	.217-11	22822	22822	23015	169
"	PECE	"	2^{-8}	22791	45582	46052	305
"	PECEC	"	2^{-8}	22791	45582	46052	305
mod. PEC	"	2^{-8}	.597-10	5987	5987	6117	191
"	PECE	"	2^{-7}	6125	12250	12256	341
"	PECEC	"	2^{-7}	6130	12260	12266	341

Table 4. Problem 4.

		starting h	relative error of y at x_{\max}	no. of integration steps	no. of successful evaluations	no. of total evaluations	no. of evaluations to start
std. PEC	$\epsilon = 10^{-6}$	2^{-5}	.240-5	745	745	773	105
"	PECE	"	2^{-4}	.162-5	680	1360	1448
"	PECEC	"	2^{-4}	.448-7	709	1418	1418
mod. PEC	"	2^{-5}	.621-6	1218	1218	1233	131
"	PECE	"	2^{-1}	.786-4	318	636	685
"	PECEC	"	2^{-4}	.148-4	309	618	644
std. PEC	$\epsilon = 10^{-13}$	2^{-9}	.114-12	9942	9942	10481	169
"	PECE	"	2^{-8}	.421-12	10303	20606	20972
"	PECEC	"	2^{-8}	.524-12	10302	20604	20972
mod. PEC	"	2^{-8}	.528-10	2717	2717	2805	191
"	PECE	"	2^{-1}	.322-10	2863	5726	5790
"	PECEC	"	2^{-7}	.277-10	2807	5586	5614

Table 5. Modified Nordsieck with $\epsilon = 10^{-13}$, $t = .95$

Problem Procedure		*	no. of integration steps	no. of successful evaluations	no. of total evaluations
1	PEC	.465-9	4185	4185	4185
1	PECE	.352-9	4166	8332	8332
1	PECEC	.289-9	4163	8326	8326
2	PEC	.796-10	817	817	817
2	PECE	.507-10	800	1600	1600
2	PECEC	.369-10	795	1590	1590
3	PEC	.179-9	4279	4279	4324
3	PECE	.315-9	4270	8540	8630
3	PECEC	.373-9	4274	8548	8638
4	PEC	.198-9	1955	1955	2002
4	PECE	.147-9	1953	3906	4008
4	PECEC	.121-9	1951	3902	4004

*The values in this column correspond to the values in the second labeled columns of Tables 1-4. The starting procedure was unchanged for these test runs.

Table 6. Modified Nordsieck with $\epsilon = 10^{-6}$, $t = .95$

Problem Procedure		*	no. of integration steps	no. of successful evaluations	no. of total evaluations
1	PEC	.232-5	2434	2434	2592
1	PECE	.695-3	460	920	922
1	PECEC	.114-3	453	906	908
2	PEC	.626-5	323	323	348
2	PECE	.973-4	83	166	166
2	PECEC	.857-4	84	168	168
3	PEC	.150-2	390	390	422
3	PECE	.254-3	377	754	826
3	PECEC	.296-3	382	764	836
4	PEC	.847-5	1244	1244	1337
4	PECE	.297-3	220	440	512
4	PECEC	.331-4	222	444	502

*The values in this column correspond to the values in the second labeled columns of Tables 1-4. The starting procedure was unchanged for these test runs.

Appendix A

Standard Nordsieck Formula

$$y(x+h) = y(x) + h(f(x) + a(x) + b(x) + c(x) + d(x) + \frac{95}{288} (f(x+h) - f^P(x+h))),$$

$$f^P(x+h) = f(x) + 2a(x) + 3b(x) + 4c(x) + 5d(x),$$

$$a(x+h) = a(x) + 3b(x) + 6c(x) + 10d(x) + \frac{25}{24} (f(x+h) - f^P(x+h)),$$

$$b(x+h) = b(x) + 4c(x) + 10d(x) + \frac{35}{72} (f(x+h) - f^P(x+h)),$$

$$c(x+h) = c(x) + 5d(x) + \frac{5}{48} (f(x+h) - f^P(x+h)),$$

$$d(x+h) = d(x) + \frac{1}{120} (f(x+h) - f^P(x+h)).$$

Modified Nordsieck Formula

$$y(x+h) = y(x) + h(f(x) + a(x) + b(x) + c(x) + d(x) + e(x) + \frac{95}{288} (f(x+h) - f^P(x+h))),$$

$$f^P(x+h) = f(x) + 2a(x) + 3b(x) + 4c(x) + 5d(x) + 6e(x),$$

$$a(x+h) = a(x) + 3b(x) + 6c(x) + 10d(x) + 15e(x) + \frac{137}{120} (f(x+h) - f^P(x+h)),$$

$$b(x+h) = b(x) + 4c(x) + 10d(x) + 20e(x) + \frac{5}{8} (f(x+h) - f^P(x+h)),$$

$$c(x+h) = c(x) + 5d(x) + 15e(x) + \frac{17}{96} (f(x+h) - f^P(x+h)),$$

$$d(x+h) = d(x) + 6e(x) + \frac{1}{40} (f(x+h) - f^P(x+h)),$$

$$e(x+h) = e(x) + \frac{1}{720} (f(x+h) - f^P(x+h)).$$

Appendix B

Characteristic Equations

Standard Nordsieck

$$\begin{aligned} \text{PEC: } z^6 - (1 + \frac{4277}{1440} s) z^5 + \frac{2641}{480} s z^4 - \frac{4991}{720} s z^3 \\ + \frac{3649}{720} s z^2 - \frac{959}{480} s z + \frac{95}{288} s = 0 \end{aligned}$$

$$\begin{aligned} \text{PECE: } z^5 - (1 + \frac{317}{240} s + \frac{36119}{41472} s^2) z^4 + (\frac{133}{240} s + \frac{26353}{20736} s^2) z^3 \\ - (\frac{241}{720} s + \frac{2071}{1728} s^2) z^2 + (\frac{173}{1440} s + \frac{12103}{20736} s^2) z \\ - (\frac{3}{160} s + \frac{4769}{41472} s^2) = 0 \end{aligned}$$

$$\begin{aligned} \text{PECEC: } z^6 - (1 + \frac{317}{240} s + \frac{81263}{82944} s^2) z^5 + (\frac{133}{240} s + \frac{50179}{27648} s^2) z^4 \\ - (\frac{241}{720} s + \frac{94829}{41472} s^2) z^3 + (\frac{173}{1440} s + \frac{69331}{41472} s^2) z^2 \\ - (\frac{3}{160} s + \frac{18221}{27648} s^2) z + \frac{9025}{82944} s^2 = 0 \end{aligned}$$

Appendix B, Characteristic Equations, continued

Modified Nordsieck

$$\begin{aligned} \text{PEC: } z^7 - (1 + \frac{33}{10} s) z^6 + \frac{1197}{160} s z^5 - \frac{17107}{1440} s z^4 \\ + \frac{8399}{720} s z^3 - \frac{1667}{240} s z^2 + \frac{665}{288} s z - \frac{95}{288} s = 0 \end{aligned}$$

PECE: Same as standard Nordsieck PECEC

$$\begin{aligned} \text{PECEC: } z^7 - (1 + \frac{317}{240} s + \frac{209}{192} s^2) z^6 \\ + (\frac{133}{240} s + \frac{2527}{1024} s^2) z^5 - (\frac{241}{720} s + \frac{325033}{82944} s^2) z^4 \\ + (\frac{173}{1440} s + \frac{159581}{41472} s^2) z^3 - (\frac{3}{160} s + \frac{31673}{13824} s^2) z^2 \\ + (\frac{63175}{82944} s^2) z - \frac{9025}{82944} s^2 = 0 \end{aligned}$$

Appendix C

Modified Nordsieck Interval Modification

	Reversal	Increase	Decrease
Replaces h	- h	βh	h/β
Replaces y	y	y	y
Replaces f	f	f	f
Replaces a	- a	βa	a/β
Replaces b	b	$\beta^2 b$	b/β^2
Replaces c	- c	$\beta^3 c$	c/β^3
Replaces d	d	$\beta^4 d$	d/β^4
Replaces e	- e	$\beta^5 e$	e/β^5

Modified Nordsieck Interpolation

Suppose z is between x and x + h

$$\text{Let } \alpha = \frac{z-x}{h}$$

$$\begin{aligned} \text{then } y(z) = & y(x) + h(\alpha f(x, y(x)) + \alpha^2 a(x) + \alpha^3 b(x) + \alpha^4 c(x) \\ & + \alpha^5 d(x) + \alpha^6 e(x)) \end{aligned}$$

$$\begin{aligned} f(z, y(z)) = & f(x, y(x)) + 2\alpha a(x) + 3\alpha^2 b(x) + 4\alpha^3 c(x) \\ & + 5\alpha^4 d(x) + 6\alpha^5 e(x) . \end{aligned}$$

For standard Nordsieck case, omit all $e(x)$ terms in the above formulas.

References

(Note. References 9 thru 11 are not cited in the text.)

1. Nordsieck, A. "Numerical Integration of Ordinary Differential Equations", *Mathematics of Computation*, v. 16, 1962, pp. 22-49.
2. Descloux, J. "Note on a Paper by A. Nordsieck", Report No. 131, Department of Computer Science, University of Illinois, Urbana, Illinois, 1963.
3. Krogh, F. T. "Predictor-Corrector Methods of High Order with Improved Stability Characteristics", *J. ACM*, v. 13, 1966, pp. 374-385.
4. Crane, R. L., and Klopfenstein, R. W. "A Predictor-Corrector Algorithm with an Increased Range of Absolute Stability", *J. ACM*, v. 12, 1965, pp. 227-241.
5. Chase, P. E. "Stability Properties of Predictor-Corrector Methods", *J. ACM*, v. 9, 1962, pp. 457-468.
6. Hall, G. "The Stability of Predictor-Corrector Methods", *The Computer Journal*, v. 9, Feb. 1967, pp. 410-412.
7. Hull, T. E., and Creemer, A. L. "Efficiency of Predictor-Corrector Procedures", *J. ACM*, v. 10, 1963, pp. 291-301.
8. Wilkinson, J. H. Rounding Errors in Algebraic Processes, Prentice-Hall, Englewood Cliffs, N. J., 1963, pp. 79-82.
9. Abramowitz, M. "Coulomb Wave Functions" in Handbook of Mathematical Functions, fifth edition, U.S. Dept. of Commerce, National Bureau of Standards, Applied Mathematics Series 55, 1965, pp. 537-554.

10. Ralston, A. "Relative Stability in the Numerical Solution of Ordinary Differential Equations", SIAM Review, v. 7, 1965, pp. 114-125.
11. Krogh, F. T. "A Test for Instability in the Numerical Solution of Ordinary Differential Equations", J. ACM, v. 14, 1967, pp. 351-354.